Indian J. Phys. 82 (3) 291 - 299 (2008)

IJP

Study of antiferromagnetism in cuprates through Raman active phonon peaks

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Abstract In the present communication we make an attempt to study the antiferromagnetism in cuprates in normal state through Raman active phonon peaks observed in the system We calculate phonon spectral density function (SDF) from $S(q,\omega) = 2\mathrm{Im}\, D_{qq}(\omega)$ The self energy reflects the properties of the ground state of the cuprates in normal state It is observed that the staggered field ($h1$) is stronger at lower temperatures and decreases as the temperature becomes higher and ultimately vanishes at the Néel temperature (t_N) The value of $h1$ at the corresponding temperatures are taken from the ($h1 \sim t$) plot and are used in the plot of SDF ~ reduced frequency The observed shift of the Raman active phonon peaks in this plot helps one to infer about the nature of antiferromagnetism in the system

Keywords Antiferromagnetic order, electron-phonon interaction Raman scattering

PACS Nos. 71 38 +i,78 30 -j

1. Introduction

An attempt is made to present a microscopic theoretical model for the cuprate systems ($R_{2-x}Ce_xCuO_4$; *R = Pr, Nd, Sm, Gd*) in presence of antiferromagnetism (AFM), the position of f-level, hybridization between f-level of the Rare-earth atom (R) and Cu d-electrons as well as phonon interaction to the hybridization in harmonic phonon vibration approximation. The underdoped systems exhibit AFM with low magnetic moments of the Cu^{2+} ion in CuO_2 plane. In our theoretical model calculation, the phonon Green's function is evaluated by Zubarev's technique [1]. We calculate phonon spectral density function (SDF) from $S(q,\omega) = -2\mathrm{Im}\, D_{qq}(\omega)$. The self energy reflects the properties of the ground state of the cuprates in normal state. It is observed that the staggered field ($h1$) is stronger at lower

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temperatures and decreases as the temperature becomes higher and ultimately vanishes at the Néel temperature (t_N). The value of $h1$ at the corresponding temperatures are taken from the ($h1 \sim t$) plot and are used in the plot of SDF reduced frequency. The observed shift of the Raman active phonon peaks [2] in this plot helps one to infer about the nature of antiferromagnetism in the system. Short communications have been reported on theoretical investigations of Raman spectra [3-5] and the study of magnetism and hybridization through ultrasonic attenuation in cuprate systems [6] (See the references there in).

2. Formalism

Simulating the strong electron correlation in the CuO plane by breaking the spin symmetry the heavy fermion behaviour of $Nd_{2-x}Ce_xCuO_4$ ($x = 0.2$) can be understood. The starting point is a lattice Hamiltonian (Fulde's model) which includes effective $Nd - Cu$ hybridization which is mediated by oxygen ions. Having to deal thereby with three strongly correlated f-electrons for Nd is a problem in itself. To avoid it, Fulde [7] has considered only one orbital per Nd ion. The present model considers AFM ground state in presence of a weak hybridization between f-electrons of the rare-earth atom and the conduction electrons of the copper atoms. Here the AFM excitation is expected to be manifested through its coupling to the phonon in the phon spectral density function.

The Hamiltonian in k-space for the cuprate system is taken as

$$\mathcal{H}_0 = \mathcal{H}_d + \mathcal{H}_s + \mathcal{H}_v + \mathcal{H}_f \tag{1}$$

where

$$\mathcal{H}_d = \sum_{k\sigma} \varepsilon_0(k) \left(a^\dagger_{k,\sigma} b_{k,\sigma} + h.c. \right) \tag{2}$$

with dispersion $\varepsilon_0(k) = -2\, t_0 \left(\cos k_x + \cos k_y \right)$

$$\mathcal{H}_s = (h/2) \sum_{k,\sigma} \sigma \left(a^\dagger_{k,\sigma} a_{k,\sigma} - b^\dagger_{k,\sigma} b_{k,\sigma} \right) \tag{3}$$

$$\mathcal{H}_v = V \sum_{k,\sigma} \left(a^\dagger_{k,\sigma} f_{1,k,\sigma} + b^\dagger_{k,\sigma} f_{1,k,\sigma} + h.c. \right) \tag{4}$$

$$\mathcal{H}_f = \varepsilon_f \sum_{k,\sigma} f^\dagger_{1,k,\sigma} f_{1,k,\sigma} \tag{5}$$

$\mathcal{H}_d$, $\mathcal{H}_s$, $\mathcal{H}_v$ and $\mathcal{H}_f$ are conduction electron, staggered field, hybridization interaction and f-electron Hamiltonian respectively. Here $a^\dagger(a), b^\dagger(b)$ are creation (annihilation) operators for the $d_{x^2-y^2}$ conduction electrons on copper sub-lattices 1 and 2 respectively

and $f^{\dagger}$ (f) are those for the f-electrons. The Fourier transformed electron-phonon interaction Hamiltonian is

$$\mathcal{H}_{e\,p} = \sum_{k,q,\sigma} f(q)\left[\left(a^{\dagger}_{k+q\,\sigma} f_{1\,k,\sigma} + b^{\dagger}_{k+q\,\sigma} f_{1,k\,\sigma}\right) + h.c.\right] A_q \tag{6}$$

with $h.c. = \left(f^{\dagger}_{1\,k+q\,\sigma} a_{k,\sigma} + f^{\dagger}_{1,k+q,\sigma} b_{k,\sigma}\right)$ and $A_q - b_q + b^{\dagger}_{-q}$ where $b_q\left(b^{\dagger}_q\right)$ are annihilation (creation) operators for phonon with wave vector q and $f(q)$ is the electron-phonon coupling constant The free phonon Hamiltonian with phonon energy ω_q is written as $\mathcal{H}_p - \sum_q \omega_q\, b^{\dagger}_q\, b_q$. Hence the total Hamiltonian of the system is described by –

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{e-p} + \mathcal{H}_p . \tag{7}$$

3. Calculation of renormalized phonon energy

The double time phonon Green function of Zubarev [1] type is defined as

$$D_{q\,q}(t - t') = \ll A_q(t);\, A_q(t') \gg = -i\Theta(t - t') < \left[A_q(t),\, A_q(t')\right] > . \tag{8}$$

Applying Dyson approximation, the phonon Green function can be written as

$$D_{q\,q}(\omega) - \left(\omega_q/\pi\right)\left[\omega^2 - \omega_q^2 - \sum_q(\omega)\right. \tag{9}$$

where phonon self energy is given by

$$\sum_q(\omega) = 4\pi\, f^2(-q)\,\omega_q\, \chi_{qq}(\omega) \tag{10}$$

$$\chi_{qq'}(\omega) = \sum_{k\,k'\,\sigma\,\sigma'}\left[\Gamma_3 + \Gamma_4 + \Gamma_5 + \Gamma_6\right] \tag{11}$$

$\Gamma_i(k,k',q,q',\omega)$'s ($i$ = 3 to 6) represent the electron response functions They are defined by dropping k,k',q,q' and ω as

$$\Gamma_3(\omega) = \left\langle\left\langle \alpha^a + \alpha^b;\, \beta^a \right\rangle\right\rangle ;$$

$$\Gamma_4(\omega) = \left\langle\left\langle \alpha^a + \alpha^b;\, \beta^b \right\rangle\right\rangle ;$$

$$\Gamma_5(\omega) = \left\langle\left\langle \alpha^c + \alpha^d;\, \beta^a \right\rangle\right\rangle ;$$

$$\Gamma_6(\omega) = \left\langle\left\langle \alpha^c + \alpha^d;\, \beta^b \right\rangle\right\rangle \tag{12}$$

where

$$\alpha^a \equiv a^{\dagger}_{k\,q\sigma} f_{k\sigma}, \quad \alpha^b \equiv f^{\dagger}_{k-q\sigma} a_{k\sigma}$$

$$\alpha^c = b^{\dagger}_{k\,q\sigma} f_{k\sigma}, \quad \alpha^d \equiv f^{\dagger}_{k\,q\sigma} b_{k\sigma} \tag{13}$$

$$\beta^d = a^{\dagger}_{k\,q\sigma} f_{k\sigma} + f^{\dagger}_{k\,q\sigma} a_{k\sigma}$$

$$\beta^b \equiv b^{\dagger}_{k\,q\sigma} f_{k\sigma} + f^{\dagger}_{k\,q\sigma} b_{k\sigma} \tag{14}$$

We make some approximations, while calculating the electron response function keeping the essential physics intact We use certain decoupling schemes for the higher order Green's functions such that all the physical parameters like f-level, staggered magnetic field, hybridization term (~ V^2) and phonon coupling term are retained. The limit of zero wave vector ($q \to 0$) and finite temperature are considered in evaluating the response function

4. Expression for the spectral density function

The spectral density function is written as $S(q,\omega) = -2\mathrm{Im}\, D_{qq}(\omega + i\eta)$

$$S(0,\omega) \quad \frac{2\,\omega_0^2\, B_1}{A_1^2 + B_1^2} \tag{15}$$

where

$$A_1 \quad \left[\omega^2 - \omega_0^2\,(1 + 4\,A_2)\right]$$

$$B_1 - \left[2\eta\,\omega \quad 4g\,\omega_0^2\, B_2\right]$$

A_2 and B_2 are written as

$$A_2 = g\int_{W/2}^{W/2} dx_0\; A_3(\epsilon_k, \omega);$$

$$B_2 = g\int_{W/2}^{W/2} dx_0\; B_3(\epsilon_k, \omega) \tag{16}$$

where

$$A_3(\epsilon_k, \omega) = \frac{1}{D_{12}}\left[A_{16}P_1 f(\omega_1) + A_{17}Q_1 f(\omega_2) + A_{18}R_1 f(\omega_3)\right]$$

$$B_3(\varepsilon_k, \omega) = \frac{1}{D_{12}}\left[B_{16}P_1 f(\omega_1) + B_{17}Q_1 f(\omega_2) + B_{18}R_1 f(\omega_3)\right]$$

and A_{16}, A_{17}, A_{18}, B_{16}, B_{17}, B_{18}, D_{12}, P_1, Q_1 and R_1 are expressed in terms of other known dimensionless parameters. Here $f(\omega_i)$ are the Fermi functions which are in turn functions of quasi-particle energies ω_i with $i = 1$ to 3 Different parameters used in the above expressions are made dimensionless by dividing them by hopping integral $2t_0$, where the width of the conduction band is $W = 8t_0$.

Different parameters involved are made dimensionless by dividing them by hopping integral $2t_0$, where the width of the conduction band in $W = 8t_0$. Those are –

$$g = f^2(0)\, N(0)/\omega_0\ ;\ d = \varepsilon_f/2t_0\ ;\ c = \omega/2t_0$$

$$v = V/2t_0\ ;\ e = \eta/2t_0\ ;\ p = \omega_0/2t_0$$

$$\bar{\omega} = c/p\ ;\quad x_0 = \varepsilon_0(k)/2t_0\ ,\quad h1 = h/2t_0\ ,\quad t - k_B T/2t_0$$

where k_B is the Boltzmann constant And other variables are

$$x = \left\{x_0^2 + \left(h1^2/4\right)\right\}^{1/2},\quad \tilde{\Delta} = \left[\left(x-d\right)^2 + 8\,V^2\right]^{1/2}$$

$$\tilde{\omega}_1 = -x_0\ ;\ \tilde{\omega}_{23} = \left(x + d \pm \tilde{\Delta}\right)/2 \tag{17}$$

5. Results and discussion

The Figure 1 shows the temperature dependence of the staggered field $h1$ corresponding to the Néel temperature $t_N \simeq 0.1\,(T_N \simeq 250\,\mathrm{K})$, $h1\,(T = 0) \simeq 0.35$, and anti-ferromagnetic

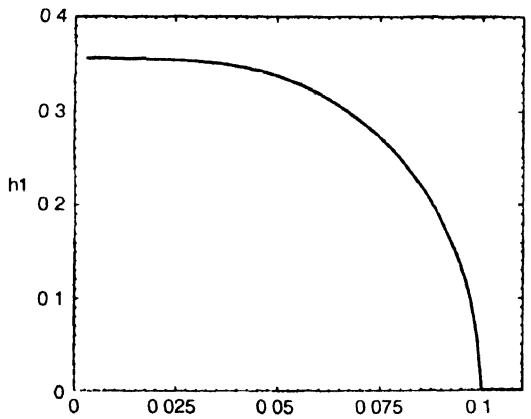

Figure 1. The plot of staggered field $h1$ *vs* temperature t for fixed values of position of f-level d = 0 06, hybridization v = 0 015

(AFM) coupling strength λ_2 = 0.320522 This represents well the normal AFM state of the cuprate system described by Brugger *et al* [8] . From this plot, we have chosen bare $h1$ = 0.195 at temperature t = 0 09 We want to study normal state Raman spectra at t = 0 09 (T = 225K) with weak hybridization v = 0.015 and f-level position d = 0.06 *i e* close to Fermi level The electron-phonon coupling parameter g = 0.025, the bare phonon frequence p = 1 0 and the finite spectral width e = 0.018 are same for all the Figures

In Figure 2, the phonon spectral density function (SDF) is plotted against the reduced phonon frequency $\tilde{\omega}$ ($= \omega/\omega_0$) for fixed values of d, $h1$, g, p, e, and t for normal state of the cuprate systems Here we observe five peaks

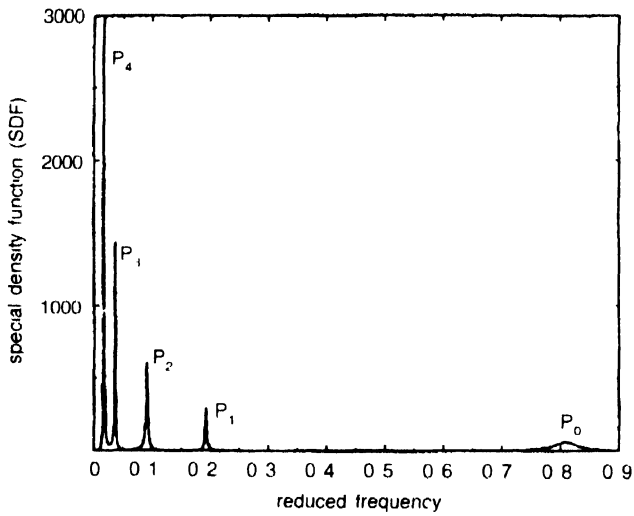

Figure 2. The plot of spectral density function (SDF) *vs* reduced frequency ($\tilde{\omega}$) for finxed values of temperature t = 0 09, position of *f*-level d = 0 06, hybridization v = 0 015, staggered field $h1$ = 0 195

The peak centered at $\tilde{\omega} = 0.81$ is denoted as P_0 and it corresponds to the renormalized bare phonon frequency of the cuprate systems for q = 0 phonon The other four peaks centered at frequencies $\tilde{\omega} = 0.193$, 0.09, 0.036 and 0.016 are denoed as P_1, P_2, P_3 and P_4 respectively. In absence of electron-phonon coupling (g = 0), the phonon self-energy is zero. Hence we observe the phonon peak P_0 at frequency $\tilde{\omega} = 1$ which corresponds to bare phonon frequency ω_q at q = 0. When the phonon coupling g is increased, the phonon self energy increases and hence it renormalises the phonon frequency.

The effect of staggered magnetic field $h1$ at different temperatures on Raman active modes is depicted in Figure 3. From Figure 1, it is observed that the staggered field $h1$ becomes stronger at lower temperatures and decreases towards high temperatures and ultimately vanishes at Néel temperature t_N. The $h1$ values are taken from Figure 1 at the corresponding temperatures and the SDF is plotted as shown in Figure 3. It is observed that all the peaks from P_1 to P_4 shift towards lower frequencies at temperature increases and correspondingly staggered field decreases. Ultimately, when temperature (t) attains t_N and higher values, all the peaks vanish except the peak P_2. Because, in non-magnetic

phase ($h1=0$), only the phonon assisted f-electron peak P_2 exists at frequency $2d$ (with f-level set at $d = 0.06$) [Not shown in Figure 3)

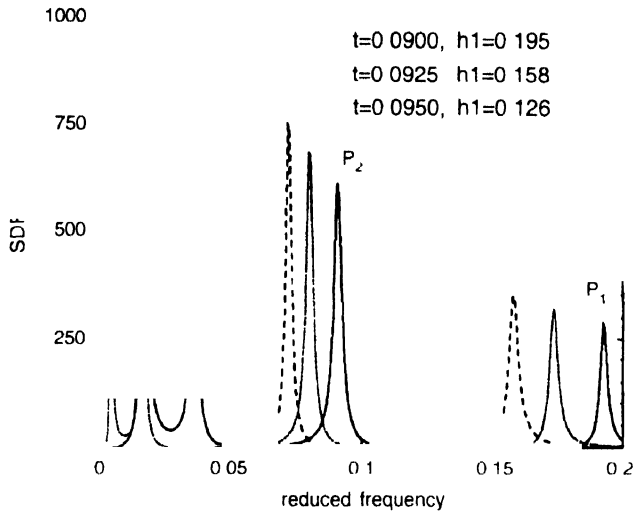

Figure 3 The plot of spectral density function (SDF) *vs* reduced frequency (ω) for fixed values of position of f-level d = 006, hybridization v = 0 015 and for different values of temperature t = 0 0900 0 0925 0 0950 with the corresponding values of staggered field $h1$ obtained from Figure 1

6. Conclusion

We report here a microscopic theory to study the antiferromagnetism through Raman spectra of cuprate systems in their normal state. the phonon spectral density function is given by $S(q,\omega) = -2ImD_{qq}(\omega + i\eta)$. The results are computed numerically and discussed The spectral density function (SDF) is calculated at room temperature and plotted by varying the staggered field ($h1$) and temperature (t) of the system Normally the SDF shows four phonon excitation peaks centered at frequencies $\tilde{\omega} \simeq 0\ 193$, 0 09, 0 036 and 0 016 denoted as P_1, P_2, P_3 and P_4 respectively In addition to a renormalised bare phonon frequency of the cuprate systems for long wave length ($q = 0$) phonon appears at peak P_0 with frequency $\tilde{\omega} = 0.81$ This frequency is softened considerably in presence of electron-phonon interaction with weak coupling $g \simeq 0.025$. This magnitude of the weak coupling is in agreement with the experimental observations for the cuprate systems $R_{2-x}M_xCuO_4$. This weak coupling is inferred from the small value of the isotope exponent of the cuprates. The variation in the magnitude of staggered field gap at different temperatures can be visualized through the shifts in the peaks P_1 to P_4 as observed from Figure 3.

Acknowledgments

The authors would like to thank the U.G.C., New Delhi for providing financial assistance vide letter No : F-PSO-35/98-99(ERO) Dated : 25.2 1999 They gratefully acknowledge the research facilities offered by the Institute of Physics, Bhubaneswar, Orissa, India

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